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<p>Research performed on this contract during the period 12/1/86-11/30/88 is described. It involves solvent dynamics in electron transfer reactions (Debye solvents and vibrational effects; non-Debye solvents), the early electron transfer steps in bacterial photosynthesis, and the use of artificial intelligence searching methods to treat many-quantum state problems in dynamics. These results were described in seven Technical Reports, published in various journals.</p>			
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# OFFICE OF NAVAL RESEARCH

Contract N00014-87-K0064

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## FINAL REPORT

by

**R. A. Marcus, Principal Investigator**

**California Institute of Technology  
A. A. Noyes Laboratory of Chemical Physics  
Pasadena, CA 91125**

**July 24, 1989**

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## Research Accomplished

During the tenure of this contract research was performed on a number of aspects of electron transfer reactions (solvent dynamics including vibrational effects, non-Debye solvent dynamics, early steps in bacterial photosynthesis) and of the use of artificial intelligence searching methods, the latter, in part, as a prelude to our current study of electron transfer reactions in structurally complicated systems such as proteins. Seven Technical Reports were issued during this period, listed below, and research on several topics was initiated: the study of the relation between charge transfer absorption and fluorescence spectra and the inverted region, a "nonadiabatic/adiabatic" coherent mechanism for electron transfers, and electron transfers between two immiscible-liquid phases and between a semiconductor and an electrolyte.

## ONR Technical Reports

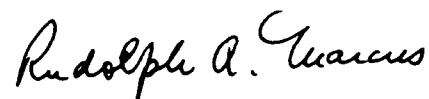
- No. 1.     Dynamical Effects In Electron Transfer Reactions. II. Numerical Solution, W. Nadler and R. A. Marcus, *J. Chem. Phys.* **86**, 3906 (1987).
- No. 2.     Recent Developments in Electron Transfer Reactions, R. A. Marcus, *Nouveau J. Chim.* **11**, 79 (1987).
- No. 3.     Some Recent Developments in Electron Transfer: Charge Separation, Long Distances, Solvent Dynamics and Free Energy Aspects, R. A. Marcus in "Supramolecular Chemistry, V. Balzani, ed. (D. Reidel, Dordrecht, 1987), *NATO ASI SER., SER. C*, **214**, 45 (1987).
- No. 4.     Non-exponential Time-Behavior of Electron Transfer in an Inhomogeneous Polar Medium, W. Nadler and R. A. Marcus, *Chem. Phys. Lett.*, **144**, 24 (1988)
- No. 5.     Application of Artificial Intelligence Methods to Intramolecular Dynamics Calculations, S. M. Lederman, S. J. Klippenstein and R. A. Marcus, *Chem. Phys. Lett.*, **146**, 7 (1988)

- No. 6. An Internal Consistency Test and its Implications for the Initial Steps in Bacterial Photosynthesis, R. A. Marcus, *Chem. Phys. Lett.*, **146**, 13 (1988)
- No. 7. Early Steps in Bacterial Photosynthesis. Comparison of Three Mechanisms. R. A. Marcus in "The Photosynthetic Bacterial Reaction Center – Structure and Dynamics," NATO ASI Series, Series A: Life Sciences, J. Breton and A. Vermeglio, eds. (Plenum, New York, 1988), p. 389.

### Research Personnel

The research personnel included Dr. W. Nadler and two graduate students, S. Klippenstein and S. Lederman, who have now received their Ph.D.'s at this Institute.

Respectfully submitted,

A handwritten signature in cursive script that reads "Rudolph A. Marcus".

R. A. Marcus  
Principal Investigator